

DOUBLE SIMPLE-HARMONIC-OSCILLATOR FORMULATION
OF THE THERMAL EQUILIBRIUM OF A FLUID
INTERACTING WITH A COHERENT SOURCE OF PHONONS

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ABSTRACT

A formulation is given for a collection of phonons (sound) in a fluid at a non-zero temperature which uses the simple harmonic oscillator twice; one to give a stochastic thermal "noise" process and the other which generates a coherent Glauber state of phonons. Simple thermodynamic observables are calculated and the acoustic two point function, "contrast" is presented. The role of "coherence" in an equilibrium system is clarified by these results and the simple harmonic oscillator is a key structure in both the formulation and the calculations.

1. Introduction

The problem of understanding the thermal properties of a radiation field in a finite volume is both old and subtle.¹⁻³ Here a sound wave propagating in a water will be studied and the key issue will be the interaction of the sound radiation with the fluid matter and with the walls of the container. The time scales of sound waves, $\nu = 20 - 2 \times 10^9 Hz$, and those of the water molecules lead to adiabatic (isentropic, if approximately reversible) thermodynamic processes rather than constant temperature transitions.⁴ This work is a special case of a project by one of us (AVN) which addresses the full nonlinear problem of bubble formation by sound waves. The linearized problem will be studied here, where the fluid has a coherent interaction with the sound radiation and an incoherent, or stochastic, interaction with the reservoir.

The harmonic oscillator has played a central role in the coherent states⁶⁻¹¹ and will be used for the coherent (Poisson) process describing the phonon radiation the sound field. Since the reservoir is incoherent the total interaction with the fluid is partially coherent.^{14,15} The reservoir is analogous to Feynman's rest of the universe¹² and Han, Kim and Noz¹³ have shown the relation of this idea to quantum squeezed states and time-uncertainty.

The model presented here will use the simple-harmonic-oscillator twice: first to generate "stochastic or chaotic" noise and second to generate a Glauber coherent state of scalar, longitudinal phonons. This is a more realistic model of noise, in that it has both coherent and a random components. It will be called partially coherent following a standard usage in quantum optics. The density, entropy free energy and a two-point function which gives the acoustic contrast are all calculated. The reason that the *SHO* is so useful is that since their Gaussian functions are dense in L^2 , quantum mechanics guarantees that the crucial interaction between the fluid and the sound radiation can be approximated by an infinite collection of oscillators. This is why the approach of Planck² was correct even though quantum mechanics was not yet created. Also, finite energy classical solutions will lie in L^2 or at least in the Sobolev space $H^1 = L^{2,1}$, which is the space where the "function"

and its "gradient" are square integrable.

In Sec. 2 the model will be presented, and the density ρ , the entropy S , the free energy F and the pair correlation function $g^{(2)}$ are calculated for both single and N-mode partially coherent states. In Sec. 3 the Conclusions and Outlook are presented.

2. The Model

In Fig. 1, a schematic is given which shows a source of sound S_0 (treated as a coherent state of phonons) a fluid F in thermal contact with the reservoir R , which is much larger than S_0 or F . In general, phonons can enter the fluid from S_0 and the fluid and reservoir can exchange particles as well as heat but all other exchanges are negligible.

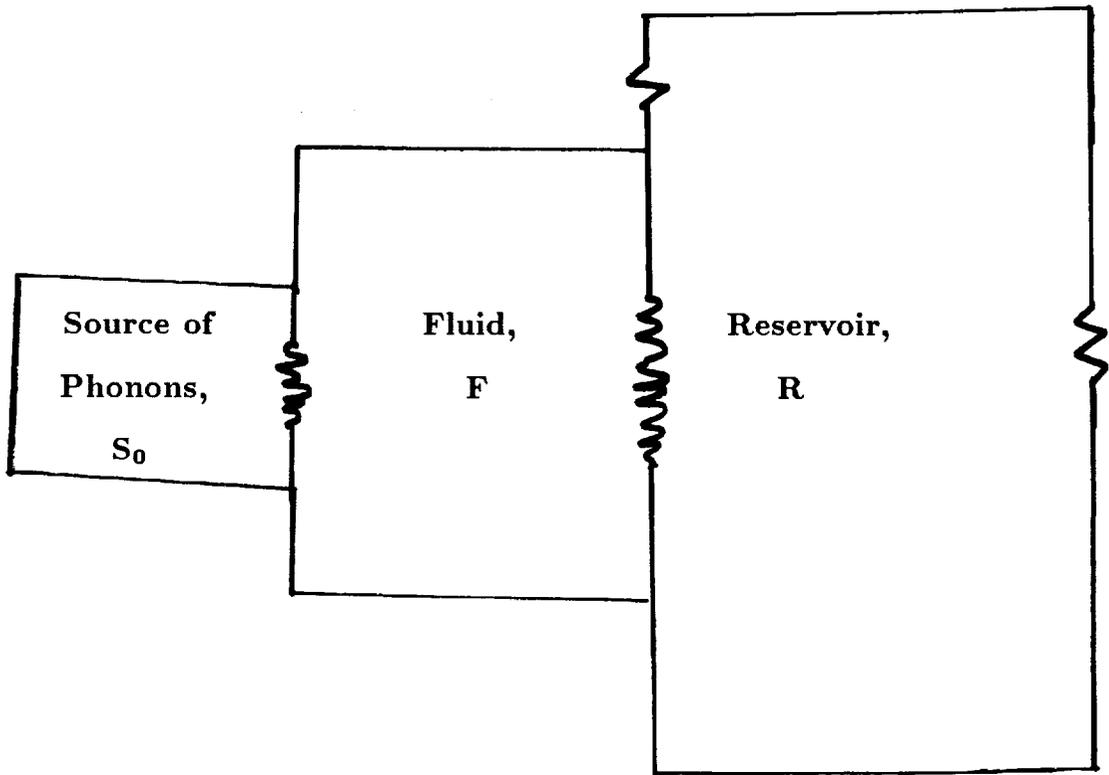


Fig. 1. Schematic of the system modeled. The source of a coherent state of phonons is S_0 , F is the stationary fluid volume and R is the reservoir which is much larger than the sum of S_0 and F . The wavy lines indicate boundaries which allow particles and energy to pass.

The idea is a modification of one due to Kaup^{16,17} that cavitons (here bubbles) are solitons (here solitary waves). In other cases, Williamsson and Wieland¹⁸, Glimm¹⁹, and others have shown that many physically interesting model solutions for plasmas and classical fluids are nonlinear, coherent excitations of the medium. The formulation given can easily be generalized to M_1 independent random components of noise and M_2 independent, coherent components. Thus, solitons and some other nonlinear modes could easily be added to the analysis.

The phonons are bosons so that their creation and destruction operators a^* , a satisfy the canonical commutation relations,

$$[a, a] = 0 = [a^*, a^*], \quad [a, a^*] = 1 \quad (1)$$

and a unique, translationally invariant Fock vacuum $|0\rangle$ exist s.t.

$$a(\vec{x}, t)|0\rangle = 0 \quad (2)$$

The asterisk power of an operator is its adjoint (a^* and a are not self-adjoint) and on a complex number is its complex conjugate. Physically, the Fock vacuum is a quantum state with no phonons. The number operator N is defined as

$$N = a^*a \quad (3)$$

and a number or Fock states is given by

$$|n\rangle = \frac{(a^*)^n}{n!} |0\rangle$$

for each $n \in \mathbb{Z}_+$, the positive integers including zero. They are eigenfunctions of the number operator with eigenvalues $n \in \mathbb{Z}_+$. The Fock representation \mathcal{H}_F of the quantum Hilbert space \mathcal{H} is the L^2 closure of the linear span of the $|n\rangle$ states. The inner-product of the Hilbert space will be written as $\langle \cdot, \cdot \rangle$ and the inner-product compatible norm is written as

$\|\cdot\| = [\langle \cdot, \cdot \rangle]^{\frac{1}{2}}$. For any complex valued $z \in C^1$ the unitary displacement operator, $U(z)$, acting on the Fock vacuum yields the minimum uncertainty coherent state $|z\rangle$ given by

$$|z\rangle = U(z)|0\rangle = e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle \quad . \quad (4)$$

The Fock vacuum is the ground state of the *SHO* for the minimum uncertainty coherent states which will be used here. In terms of c-number coordinate q and momentum p the complex number z is written as

$$z = (q, p) = q + ip \quad (5)$$

so that C^1 corresponds to the phase-space of the $(1-d)$ system. Two properties of the coherent states are that

$$a|z\rangle = z|z\rangle \quad (6)$$

and

$$\langle z_1, z_2 \rangle = e^{-\frac{1}{2}(z_1^* - z_2^*)(z_1 - z_2)} e^{-\frac{1}{2}(z_1^* z_2 - z_1 z_2^*)} \quad . \quad (7)$$

From eq. (7) it is clear that the coherent are continuous in the label z and therefore are an overcomplete family of states, *OFS*. The L^2 -closure of the linear span of the coherent states $|z\rangle$ provides a continuous representation of the physical Hilbert space which will be written as \mathcal{H}_{cs} .

A density operator is a positive, self-adjoint operator which satisfies

$$\rho^2 = \rho = \rho^* \quad . \quad (8)$$

The expected value of an observable $A = A^*$ in a state $\psi \in \mathcal{H}$ with corresponding density operator ρ_ψ can be expressed as

$$\langle A \rangle_\psi = \langle \psi, A\psi \rangle = Tr(\rho_\psi A) \quad . \quad (9)$$

And additive thermal noise can be added "by hand." The entropy of the system, S , is given by

$$S = -k_B Tr[\rho \ln \rho] \quad (10)$$

where k_B is the Boltzman constant. In information theory, one can set $k_B = 1/\ln 2$ and still use eq. (10). The entropy is obtained from maximizing eq. (10) subject to the constraints

$$\text{Tr}(\rho) = 1 \quad (11)$$

and

$$\text{Tr}(\rho N) = c \quad (12)$$

where $c \in \mathbb{R}^+$ is a parameter which labels the strength of the thermal state. If the thermal noise is Gaussian, its density operator can be expressed as

$$\rho(c) = \frac{1}{\pi c} \int d^2 z e^{-|z|^2/c} |z\rangle\langle z| \quad (13)$$

In \mathcal{H}_F this can be re-written as

$$\rho(c) = \frac{1}{\pi c} \int d^2 z e^{-|z|^2/c} e^{-|z|^2} \sum_{n=0}^{\infty} \frac{z^{2n}}{n!} |n\rangle\langle n| \quad (14)$$

Using Fubini's theorem to interchange the integral and the infinite sum and then expressing z in plane polar coordinates gives

$$\rho(c) = \sum_n \left[\frac{1}{(c+1)(1+1/c)^{n+1}} |n\rangle\langle n| \right] \quad (15)$$

in the Fock representation. A similar calculation of the entropy gives

$$S = k_B [(c+1)\ln(c+1) - c \ln(c)] \quad (16)$$

This sort of calculation was given by Glauber¹⁰, Wolf¹⁴, Sudarshan¹⁵ and probably by others. The n^{th} -order correlation function, $g^{(n)}(X_1, \dots, X_n)$, with Glauber's normalization convention is

$$g^{(n)}(X_1, \dots, X_n) := \frac{G^{(n,n)}(X_1, \dots, X_n)}{\prod_{k=1}^n [G^{(1,1)}(X_k, X_k)]^{1/2}} \quad (17)$$

where the $G^{(i,j)}$'s are Green's functions or correlation functions. This is a quantum generalization of the classical coherence degree γ of Born and Wolf.²⁰ The visibility v of a two-slit interference pattern is related to γ_{12} by

$$v = 1 \pm |\gamma_{12}(\varphi)| \quad (18)$$

which physically represents the extremes in intensity. For the two-point function, $g^{(2)}(\cdot)$, the $G^{(nm)}$'s are chosen s.t

$$G^{(2)}(\rho) = \frac{\text{Tr}[\rho N(N-1)]}{\text{Tr}(\rho N)^2} - 1 \quad . \quad (19)$$

This object is proportional to Glauber's $g^{(2)}$ in ref. (10) but is not equal to his function because of different normalizations..

In the case of the thermal states, the Fock representation of $g^{(2)}$ for $n \neq 0$ is given by

$$g_F^{(2)}(|n \rangle \langle n|) = \frac{\text{Tr} \left[|n \rangle \langle n| N(N-1) \right]}{\left[\text{Tr}(|n \rangle \langle n| N) \right]^2} - 1 = \frac{n^2 - n}{n^2} - 1 = -\frac{1}{n} \quad . \quad (20)$$

A coherent state is very different from eq. (20) since

$$g_{cs}^{(2)}(|z \rangle \langle z|) = \frac{\text{Tr} \left[|z \rangle \langle z| N(N-1) \right]}{\left[\text{Tr}(|z \rangle \langle z| N) \right]^2} - 1 = 0 \quad , \quad (21)$$

i.e. the Glauber state is *perfectly coherent*.

For the thermal states, not surprisingly, $g^{(2)}$ has the opposite behavior from eq. (21) because

$$\begin{aligned} g_{Th}^{(2)}[\rho_{Th}(c)] &= \frac{\text{Tr} \left[\sum_n \left(\frac{1}{c+1} \right) \left(\frac{1}{1+1/c} \right)^{n+1} |n \rangle \langle n| N(N-1) \right]}{\left\{ \text{Tr} \left[\sum_n \left(\frac{1}{c+1} \right) \left(\frac{1}{1+1/c} \right)^{n+1} |n \rangle \langle n| N \right] \right\}^2} \\ &= \frac{\sum_n \left[\left(\frac{1}{c+1} \right) \left(\frac{1}{1+1/c} \right)^{n+1} n(n-1) \right]}{\left[\sum_n \left(\frac{1}{c+1} \right) \left(\frac{1}{1+1/c} \right)^{n+1} n \right]^2} - 1 \quad . \end{aligned} \quad (22)$$

Defining

$$f_n(c) := \frac{1}{(c+1)} \left(\frac{1}{1+1/c} \right)^{n+1},$$

eq. (22) becomes

$$g_{Th}^{(2)}(c) = \frac{\sum_n f_n(c)(n^2 - n) - \sum_n f_n(c)n}{\left[\sum_n f_n(c)n \right]^2} = 1, \quad (23)$$

which is *perfectly incoherent*. Now a partially coherent state has a density operator which is given by

$$\rho(z; c) = U(z)\rho_{Th}(c)U^*(z) = \frac{1}{\pi c} \int d^2 x e^{-|x|^2/c} |z+x\rangle\langle z+x|. \quad (24)$$

A calculation similar to the one outlined between eqs. (14) and (15) gives

$$\begin{aligned} Tr[\rho(z; c)N] &= Tr \left\{ \frac{1}{c\pi} \int d^2 x e^{-|x|^2/c} \sum_m n \left[\frac{(z+x)^n (z^*+x^*)^m}{n!m!} e^{-|z+x|^2/2} |n\rangle\langle n| N f_{mn} \right] \right\} \\ &= |z|^2 + c. \end{aligned} \quad (25)$$

It is straightforward to calculate the entropy of the partially coherent state from

$$\begin{aligned} S(z; c) &= -k_B Tr \left[\rho(z; c) \ln(\rho(z; c)) \right] \\ &= -k_B Tr \left[\rho(c) \ln(\rho(c)) \right] \\ &= S(c) \\ &= k_B [(c+1)\ln(c+1) - c \ln(c)], \end{aligned} \quad (26)$$

where eq. (16) was used in the last two equalities. The pair correlation function, $g^{(2)}$, of a partially coherent state is given by

$$g_{cs}^{(2)}[\rho(z; c)] = 1 - \left(\frac{|z|^2}{c + |z|^2} \right)^2, \quad (27)$$

in the coherent state basis. Let $m \geq n$ with $m, n \in \mathbb{Z}_+$ and form the $nm^t h$ matrix element of the partially coherent density operator as

$$\begin{aligned} \langle n, \rho(z; c) m \rangle &= e^{-|z|^2/(1+c)} \frac{1}{1+c} \frac{1}{(1+1/c)^{(m+n/2)}} \\ &\cdot \left(\frac{n!}{m!} \right)^{1/2} \left(\frac{z}{\sqrt{c(1+c)}} \right)^{n-m} P_{n-m}^m \left(\frac{|z|^2}{c(1+c)} \right), \end{aligned} \quad (28)$$

where $P_l^m(r)$ is the polynomial given by

$$P_l^m(r) = \sum_{k=0}^m \frac{m!}{k!(l+k)!(m-k)!} r^k .$$

The thermal or noise density can be found from the $c \rightarrow 0$ limit of the previous equation and is given by the familiar expression

$$\langle n, \rho(z; 0) \rangle = e^{-|z|^2} \frac{z^n (z^*)^m}{\sqrt{n!m!}} . \quad (29)$$

By calculating another Gaussian integral, an overlap of two partially coherent states is found to be

$$\text{Tr} [\rho(z_1; c_1) \rho(z_2; c_2)] = \frac{\exp \left[\frac{|z_1 - z_2|^2}{1 + c_1 + c_2} \right]}{(1 + c_1 + c_2)} . \quad (30)$$

Clearly as $c_1 \rightarrow c_2 = c$, eq. (30) reduces to

$$\text{Tr} [\rho(0; c) \rho(0; c)] = \frac{1}{1 + 2c} . \quad (31)$$

Remark: The non-zero part of the entropy $S(c) = S(z; c)$ and the non-unit part of $\text{Tr} [(\rho(z, c))^2]$ give a measure of the magnitude of the departure from a pure coherent state. The generalization to M modes, with M a positive, finite integer is straightforward. Let (a, z) be $M \times 1$ matrices, let (a^*, z^*) be $1 \times M$ matrices, 1 the $M \times M$ unit matrix where $k = 1, 2, \dots, M$ labels which mode. Let \mathcal{B} be a given non-singular, Hermitian, $M \times M$, positive, covariance matrix and express the M -mode Fock state as

$$|n_1, \dots, n_m \rangle = \prod_{k=1}^M \frac{(a^*)^{n_k}}{\sqrt{n_k!}} |0 \rangle , \quad (32)$$

where n_k is the occupation number of the k^{th} -mode. The M -mode thermal density operator is given by

$$\rho_{Th}(\mathcal{B}) = \frac{e^{-a^* \ln(1 + \mathcal{B}^{-1}) a}}{\det(1 + \mathcal{B})} \quad (33)$$

$$= \frac{1}{\det(\mathcal{B})} \int \prod_{z=1} d^2 x \cdot e^{-x^* \cdot \mathcal{B}^{-1} \cdot x} |x \rangle \langle x| , \quad (34)$$

where $x = (x_1, \dots, x_M)$ is the M -component, complex, coherent state amplitude. The entropy of an M -mode phonon packet is given by

$$S(\mathcal{B}) = k_B \text{Tr}[(1 + \mathcal{B}) \ln(1 + \mathcal{B}) - \mathcal{B} \ln \mathcal{B}] = S(x; \mathcal{B}) \quad (35)$$

for both the incoherent and the partially coherent cases. The pair correlation function $g^{(2)}$ for an M -mode partially coherent system is

$$g^{(2)}(z; \mathcal{B}) = \frac{\text{Tr}[\mathcal{B} \cdot \mathcal{B} + 2z^* \cdot \mathcal{B}z]}{(\text{Tr}(\mathcal{B}) + |z|^2)^2} \quad (36)$$

which has the limits

$$g^{(2)}(0, \mathcal{B}) = 1 \quad (37a)$$

and

$$g^{(2)}(z, 0) = 0 \quad (37b)$$

To find the partition function for the partially coherent system one needs the mode energy e_k for the k^{th} -mode which is real

$$e_k = e_k^* \quad (38)$$

and the M -mode vector

$$\vec{e} = \begin{pmatrix} e_1 \\ e_2 \\ \vdots \\ e_M \end{pmatrix} \quad (39)$$

which is a vector-valued, intensive variable. The mode energies for the k^{th} mode is

$$E_k = n_k e_k = E_k^* \quad (40)$$

where n_k is the occupation number for the k^{th} mode and

$$\vec{\mathcal{E}} = (E_1, \dots, E_m) \quad (41)$$

is a real, vector-valued, extensive variable dual to eq. (39). In this more general case the density operator $\rho(z; \mathcal{B})$ which maximizes the entropy

$$S = -k_B \text{Tr}[\rho \ln \rho]$$

is subject to the constraints

$$\text{Tr}(\rho) = 1 \quad , \quad (42a)$$

$$\text{Tr}(\rho a) = z \quad , \quad (42b)$$

$$\text{Tr}(\rho a^*) = z^* \quad , \quad (42c)$$

and

$$\text{Tr}(\rho a^* \vec{e} a) = z^* \vec{e} z + \vec{e} \quad . \quad (42d)$$

Let $\vec{\beta}$ be an m -vector with the value $\beta = 1/k_B T$ for each component and express the given covariance matrix for bosons as

$$\mathcal{B} = \mathcal{B}(\beta) = (e^{-\vec{\beta} \cdot \vec{\mathcal{E}}} - 1)^{-1} = (e^{-\beta E} - 1)^{-1} \quad . \quad (43)$$

(A similar argument for Fermi-Dirac particles would replace -1 by $+1$ in eq. (43) but this is not needed here.) The partition function $Z(\beta, V)$ is now

$$Z(\beta, V) = \det \left(\frac{1}{1 - e^{-\beta E}} \right) \quad (44)$$

at thermal equilibrium and V is the volume of the fluid plus radiation. From eq. (44) all of the equilibrium thermodynamic quantities can be calculated, for example the average energy $\bar{\mathcal{E}}$ is

$$\bar{\mathcal{E}} = \frac{\sum_r E_r e^{-\beta E_r}}{z} = - \frac{\partial \ln(Z)}{\partial \beta} \quad (45a)$$

when classically

$$Z(\beta, V) = \sum_r e^{-\beta E_r} \quad (45b)$$

and in quantum statistical mechanics a Trace over matrix elements of $e^{-\beta H}$ is taken. The pressure p is

$$p = \frac{1}{\beta} \frac{\partial \ln(Z)}{\partial V} \quad (45c)$$

and the (reversible) differential work dW is

$$dW = -pdV \quad (45d)$$

and the previous equation can be used to obtain

$$dW = -\frac{1}{\beta} \frac{\partial \ln(Z)}{\partial V} dV \quad .$$

The entropy of eq. (10) can also be written as

$$S = k_B [\ln(Z) + \beta \bar{\mathcal{E}}] \quad (45e)$$

and the Helmholtz free energy is

$$F(\beta, V) = -\frac{1}{\beta} \ln[Z(\beta, V)] \quad . \quad (45f)$$

The coherent state density operator can be given as

$$\rho(z) = \det \left[(1 - e^{-\beta E}) e^{-(a^* - z^*) \beta E (a - z)} \right] \quad . \quad (46)$$

Near equilibrium, a Kubo linear response theory²¹ can be established by studying small deviations from equilibrium where the fluctuations will be equal to the dissipations. This exercise will be left to a future project.

3. Conclusions and Outlook

A two-component thermodynamics was formulated for a fluid in thermal equilibrium with a reservoir radiated by a coherent state of phonons. One future project will be to derive the Kubo fluctuation-dissipation theorem for this system, another will be to compare and contrast these results with both the Langevin equation and the stochastic quantization approaches. These future studies should illuminate (or simplify) the lattice Monte Carlo methods.

Much remains to be learned from harmonic, *SHO*, systems.

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